TUT 77 – Getting Started with OriginPro 8 (Part 2)

An introduction to OriginPro, a scientific charting package.

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Format Conventions

In this document the following format conventions are used:

Commands that you must type in are shown in a bold, Courier font.	**`WIN31`**
Menu items are given in a bold, Arial font.	**Windows Applications**
Keys that you press are given in a bold, Arial font, enclosed in angle brackets.	**<Ctrl>**

Feedback

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Print Record

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This document continues from 'Getting Started with OriginPro 8 (Part 1)'.

Task 9 Curve fitting: pre-defined

Objective To introduce the concept of curve fitting.

Instructions You will use a pre-defined function as an example.

OriginPro's curve fitting commands are located in the **Analysis > Fitting** menu. The most commonly used options have their own menu entry:

- **Linear**
- **Polynomial**
- **Exponential**
- **Sigmoidal**

The **Nonlinear Curve Fit** option gives access to over 200 pre-defined functions which are divided into the following (overlapping) categories:

- Origin Basic Functions
- Exponential
- Growth/Sigmoidal
- Hyperbola
- Logarithm
- Peak Functions
- Pharmacology
- Polynomial
- Power
- Rational
- Waveform
- Chromatography
- Electrophysiology
- Pharmacology
- Spectroscopy
- Statistics

The **Nonlinear Surface Fit** option gives access to 19 pre-defined functions.

You can also add your own functions to both the **Nonlinear Curve Fit** and **Nonlinear Surface Fit** options.

Apart from the **Linear** and **Polynomial** options, which have individual dialog boxes, curve fitting is controlled by the NonLinear Fitting (NLFit) dialog box which lets you select or define your own function, select a dataset for fitting, initialise and fix the fitting parameters, and perform an iterative fitting procedure which displays the results in the graph window. It also gives you access to more advanced features.

When OriginPro performs fitting, a fitted curve/surface and table of fitting parameters and statistical results are displayed in the graph window. A report sheet and a worksheet containing the fitted data are added to the workbook/matrix book which contains the source data.

Activity 9.1 You will consider a curve fitting session using one of the pre-defined functions:

- Open a new workbook and import the ASCII data file Exponential Decay.dat which can be found in Q:\origin8.v01\Samples\Curve Fitting (as in Activity 7.1).
- Create a scatter plot of column B from this dataset (using the **Plot > Symbol > Scatter** option).

Figure 26 shows the plot which will be used for this example.

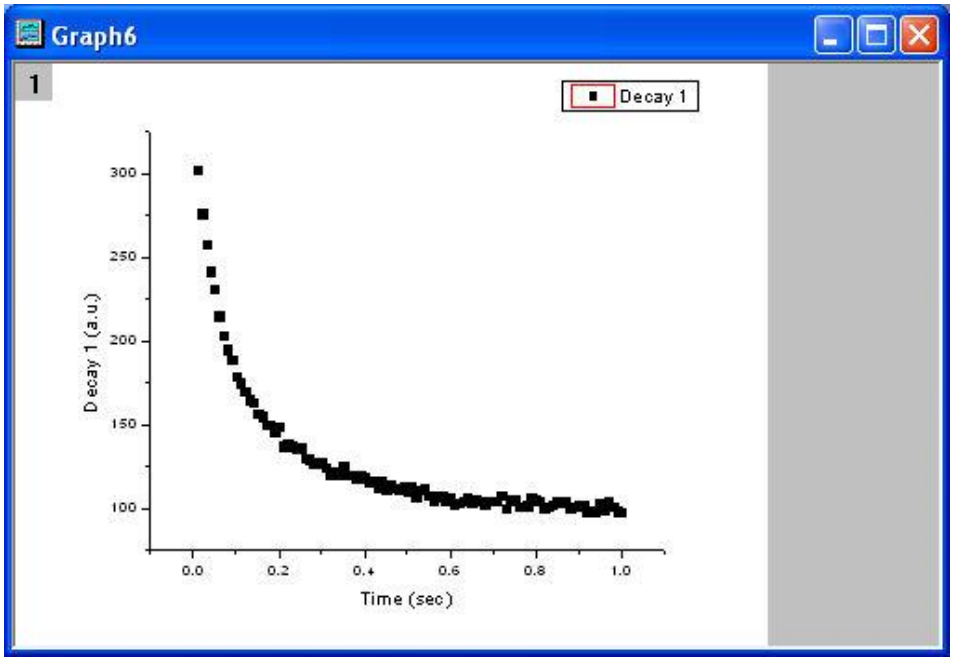


Figure 1. A scatter plot

- Click on the graph and choose **Fitting > Fit Exponential** from the **Analysis** menu to open the NLFit dialog box.

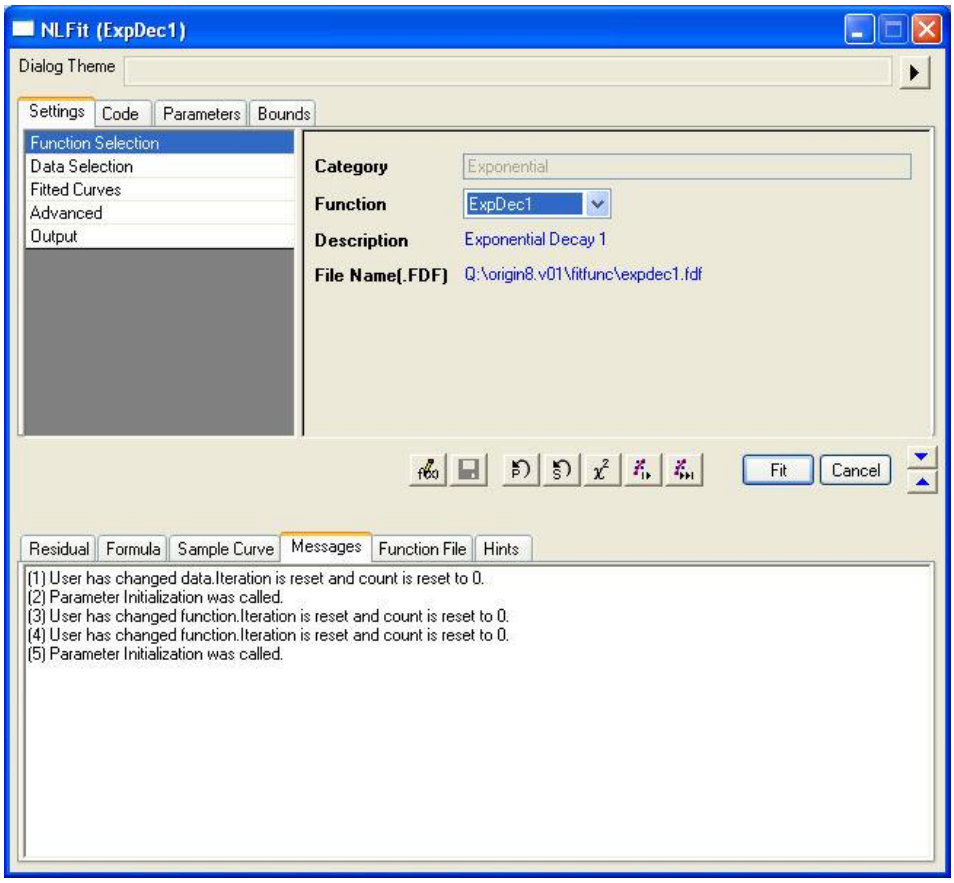


Figure 2. The NLFit dialog box

Notice that an initial fit of the default fitting function ExpDec1 has appeared in the graph window.

- Keeping this function selected, click on the 'Fit until converged' button in the NLFit dialog box, .

Look at the Messages tab at the bottom, it says that the fit has converged after 8 iterations. The fitted curve in the graph window should now fit the data better.

- Click on OK and select 'No' when asked if you want to switch to the Report Sheet.

The graph window should look as follows:

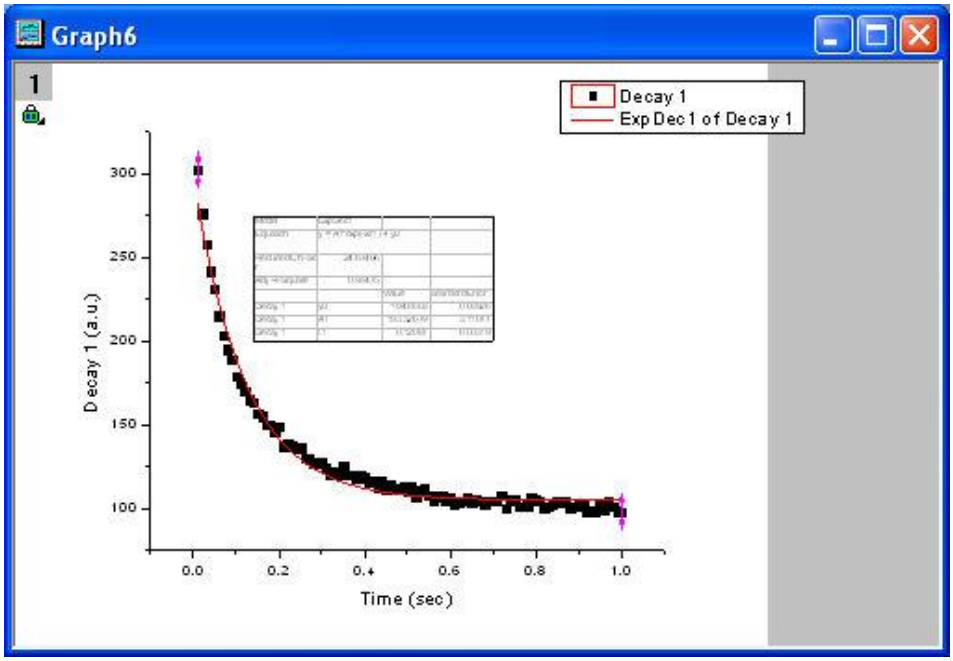


Figure 3. Exponential decay curve fitting

Details of the fitting parameters appear in the graph window, Table 1 and a report sheet which has been added to the workbook. A worksheet containing the fitted data has also been added to the workbook.

Activity 9.2 You will now choose one of the other exponential functions which can be used for fitting to perform a second fit:

- Select **Fitting > Fit Exponential > Open Dialog** from the **Analysis** menu to re-open the NLFit dialog box.
- Click on the Formula tab at the bottom to see the equation of ExpDec1:

  $$y = y0 + A*\exp(-x/t)$$

- Click on the Sample Curve tab at the bottom to see an example of this type of curve.
- Select some of the other functions and see how their formulae and curves differ.
- Choose an appropriate function to perform a second fit.
- Click on Data Selection to check that the Decay 1 data is still selected.

The Parameters tab lists the parameters whose values will be calculated during the fit. You can alter their initial values and you can fix these values if you do not wish them to change.

The Bounds tab lets you set lower and upper bound values on the parameters.

The Constraints section on the Code tab lets you set linear constraints on the parameters.

- Click on the 'Fit until converged' button.

Note that you may have to click on the 'Fit until converged' button more than once if the fitting tolerance is not reached before the maximum number of iterations have been carried out (the maximum number of iterations is specified in the Fit Control branch in the

Advanced page of the Settings tab). Also check the Messages tab at the bottom to see if there is a reason why the fit is not converging.

- Click on OK.

The graph is updated with a new fitted curve and the new fitting parameters replace the old in both the graph window and Table 1. A new report sheet and worksheet containing the fitted data are added to the workbook.

Task 10 Curve fitting: user-defined

Objective To perform curve fitting using a user-defined function.

Instructions You will use a user-defined function as an example.

Activity 10.1 You will consider a curve fitting session using a user-defined function. To try this example:

- Open a new workbook (as in Activity 7.1) and enter the data shown below.
- Create a scatter plot (as in Activity 9.1).

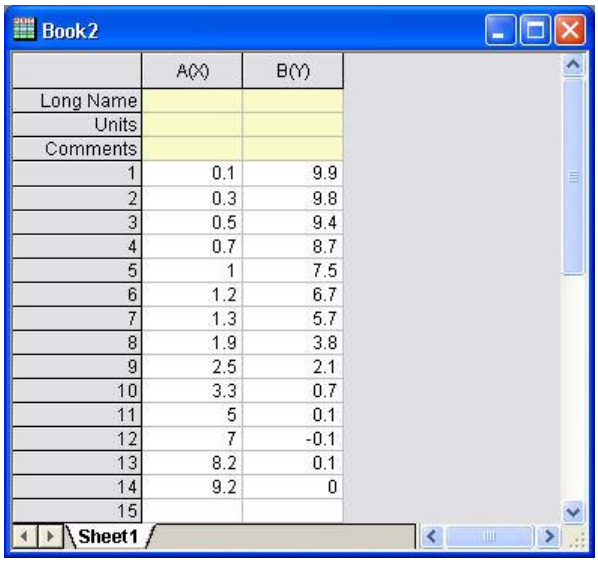


Figure 4. Entering data

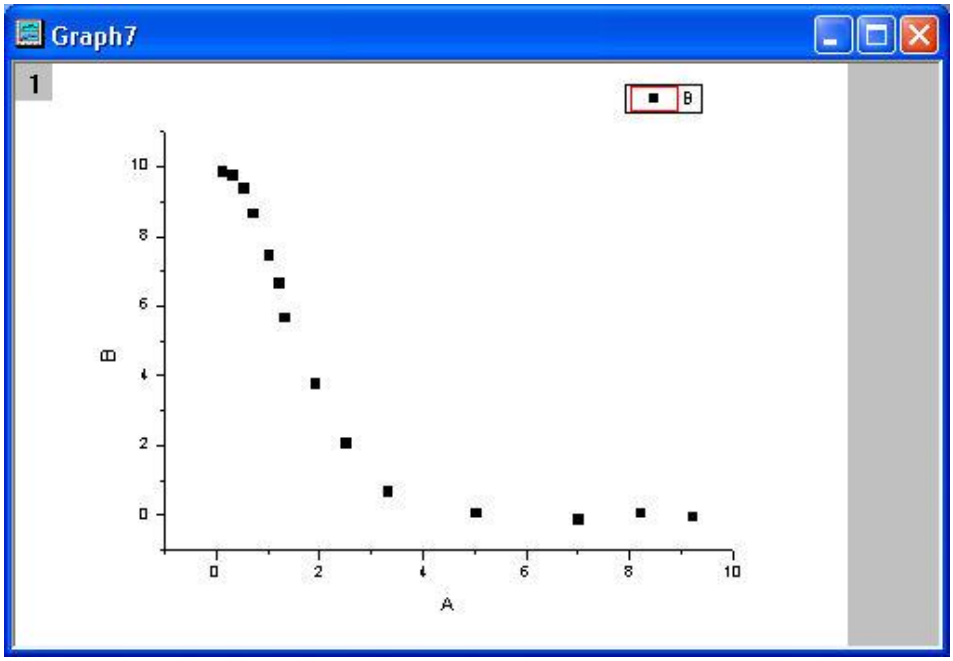


Figure 5. A scatter plot

Activity 10.2 To enter a new fitting function:

- Choose the **Fitting > Nonlinear Curve Fit** option from the **Analysis** menu.

The NLFit dialog box is displayed.

- From the Category drop-down menu, choose <New...> in the User Defined section.

The Fitting Function Organizer dialog box opens showing a NewCategory folder in which you can store your new fitting function.

- Choose to change the name of this folder by typing over the blue-highlighted text.
- Click on the New Function button.

You should see the following:

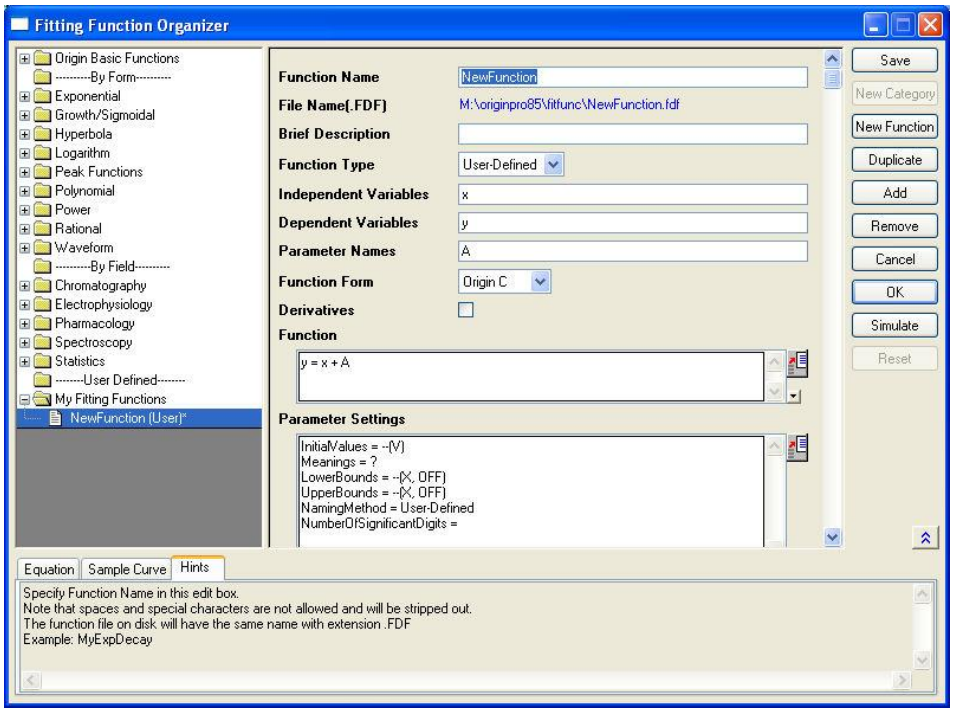


Figure 6. The Fitting Function Organizer dialog box

Notice that, as this function is in the User Defined section, it will be stored in the originpro85 folder on your M: drive.

Working from the default settings shown above:

- Choose a name for your function.
- Enter 'P1,P2,P3' in the Parameter Names section and enter the following in the Function section:

  y=P1*exp(-x^P2/P3)

- Click on next to the Parameter Settings section to open the Parameter Settings dialog box.
- For this example choose P1=7, P2=2 and P3=2 as initial parameter values:

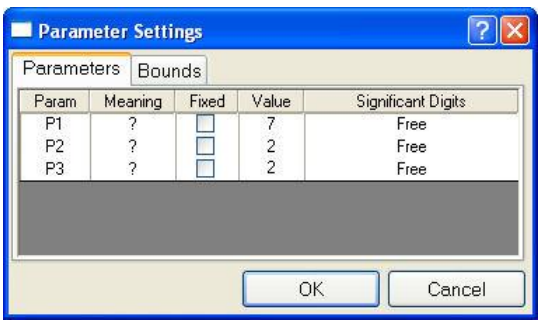


Figure 7. Setting the initial parameter values

If you want to fix the values of any of the parameters you must tick the Fixed box next to the parameters concerned. If the Fixed boxes are unticked it allows the parameters'

values to change during curve fitting iterations. The Bounds tab lets you set lower and upper bound values on the parameters.

- Click on OK.

The Fitting Function Organizer dialog box should now look as follows:

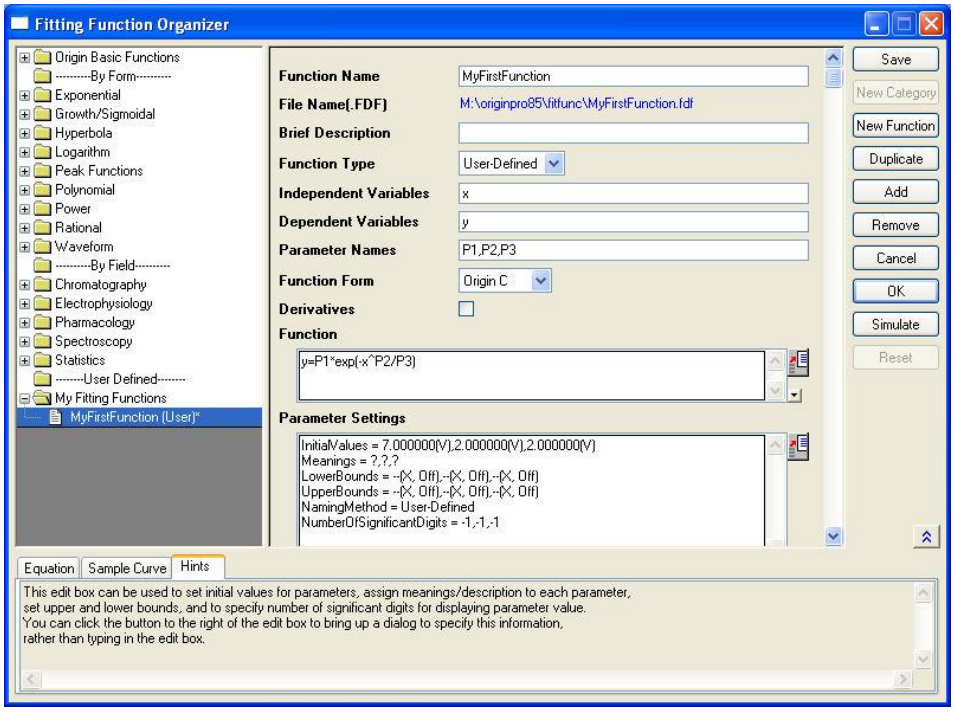


Figure 8. Creating a new fitting function

Notice that, lower down, you can also set linear constraints on the parameters.

- Click on Save to save the function and then on Cancel to return to the NLFit dialog box.

Activity 10.3 Notice that an initial fit of your fitting function has now appeared in the graph window.

- Click on the 'Fit until converged' button.

The Messages tab at the bottom says that the fit has converged after 6 iterations.

- Click on OK and select 'No' when asked if you want to switch to the Report Sheet.

The graph window should look as follows:

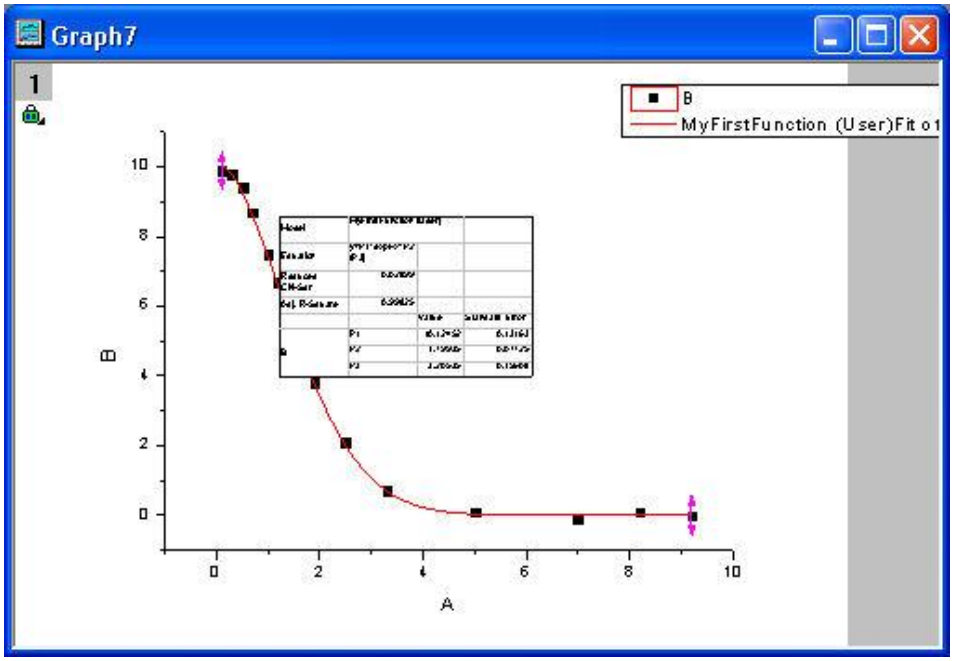


Figure 9. Fitting a user-defined function to a graph

Details of the fitting parameters appear in the graph window, Table 2 and a report sheet which has been added to the workbook. A worksheet containing the fitted data has also been added to the workbook.

Task 11 Creating a 3D graph

Objective To create a 3D graph.

Instructions You will import data into a worksheet and produce a 3D graph.

Activity 11.1 To try this example:

- Open a new workbook and import the ASCII data file 3D Scatter.dat from Q:\origin8.v01\Samples\Graphing (as in Activity 7.1).

You will work with the first three columns of data, A(X), B(Y) and C(Y). To change the association of column C to Z:

- Click on the column C(Y) heading and select the **Set as Z** option from the **Column** menu.

Activity 11.2 To plot a 3D scatter graph:

- Click on the column C(Z) heading and select **Plot > 3D XYZ > 3D Scatter**.

The data will be plotted in a new graph window and the 3D Rotation toolbar will also appear.

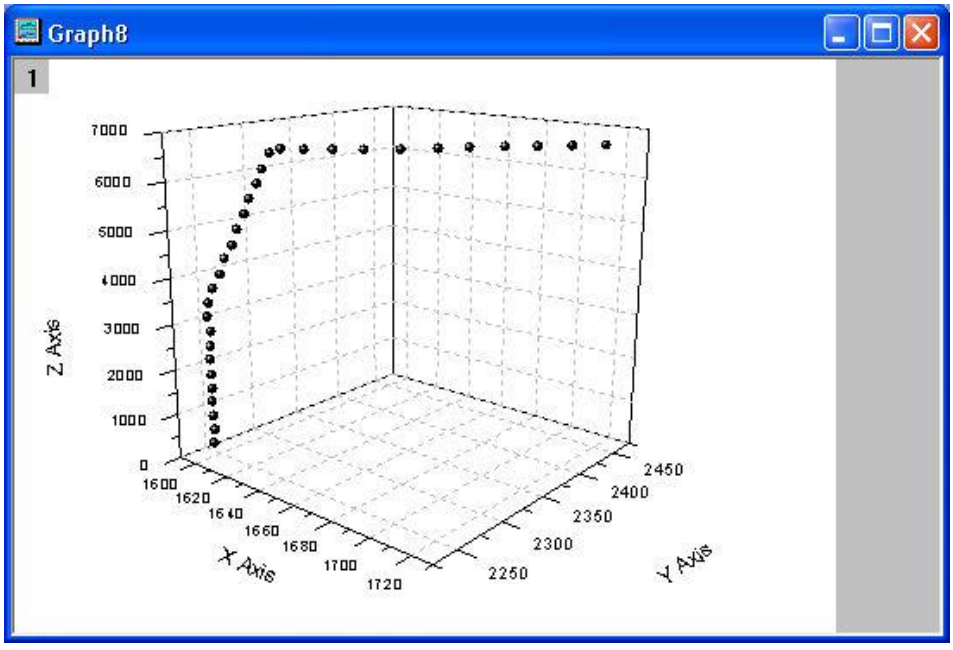


Figure 10. A 3D scatter graph

Activity 11.3 The Plot Details dialog box allows you to choose and change various parameters of a 3D scatter graph.

- Open the Plot Details dialog box by either double-clicking on a plotted data point or clicking on the **Format** menu and choosing the **Plot** option.

The following dialog box appears:

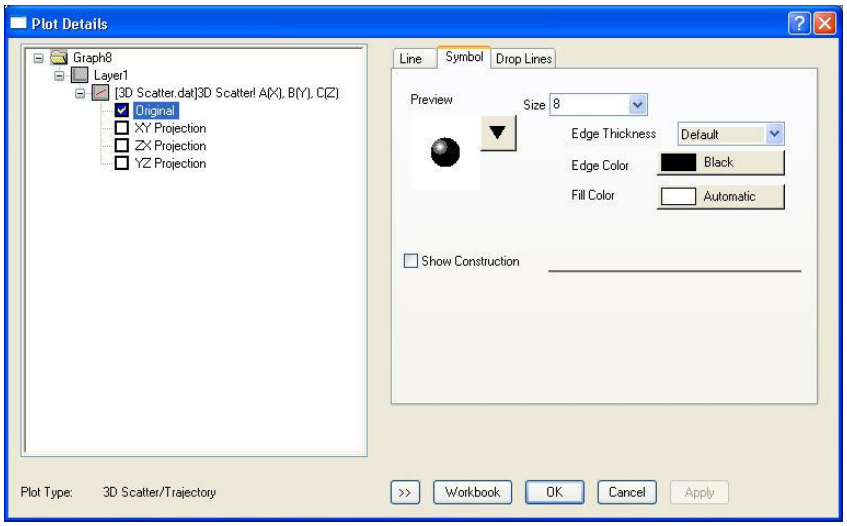


Figure 11. The Plot Details dialog box

If the left-hand side of the Plot Details dialog box looks different from above, expand the graph structure by clicking on the +'s. Make sure that Original is selected.

The display of the graph can be customised as follows:

To join the points with straight lines (a trajectory graph):

- Click on the tick box next to Connect Symbols on the Line tab. (Alternatively you could have chosen the **3D Trajectory** option, instead of the **3D Scatter** option, when creating the graph.)

To add drop lines:

- Choose the Drop Lines tab and select Parallel to Z Axis.

To remove the grid lines from all three axes:

- Click on Layer1 in the left hand side of the Plot Details dialog box and choose the Display tab.
- In the Show Elements section de-select the X Axes, Y Axes, and Z Axes options and then click on OK.

The graph should now resemble that in Figure 37.

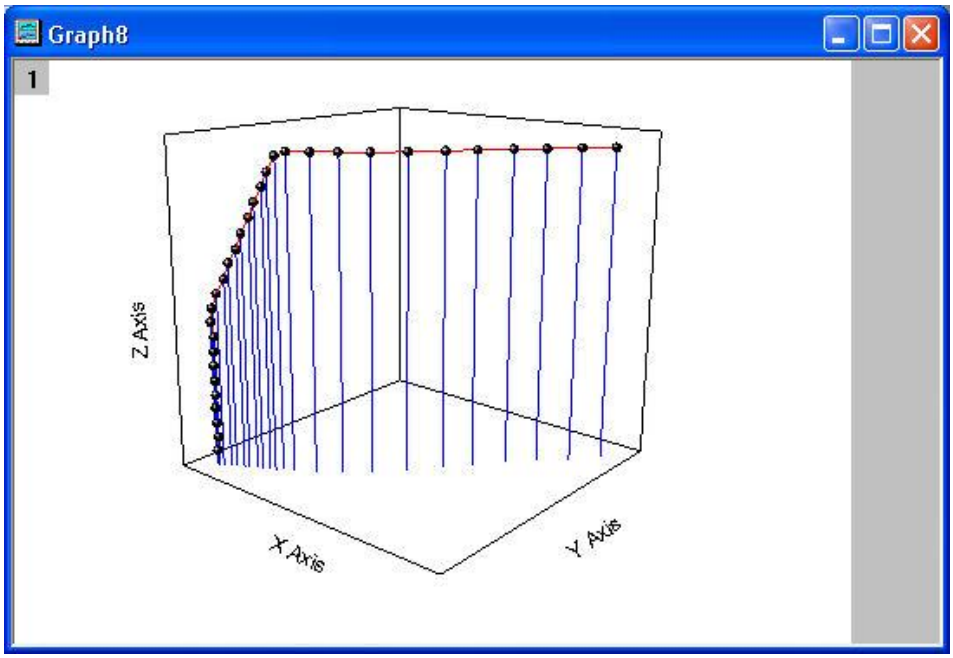


Figure 12. A trajectory graph with no grid lines

To make the points bigger and to number them:

- Re-open the Plot Details dialog box as before.
- Select Original from the left hand side of the dialog box and click on the Symbol tab.
- Choose Show Construction, Row Number Numerics, select the Outline box and choose size 12 from the drop down list.

To trace a line onto the bottom of the graph:

- Click on the XY Projection tick box in the left hand side of the Plot Details dialog box, so a tick shows.
- Click on the tick box next to Connect Symbols in the Line tab.
- Select Original from the left hand side and deselect the Parallel to Z Axis option in the Drop Lines tab.
- Click on OK.

The graph should look as follows:

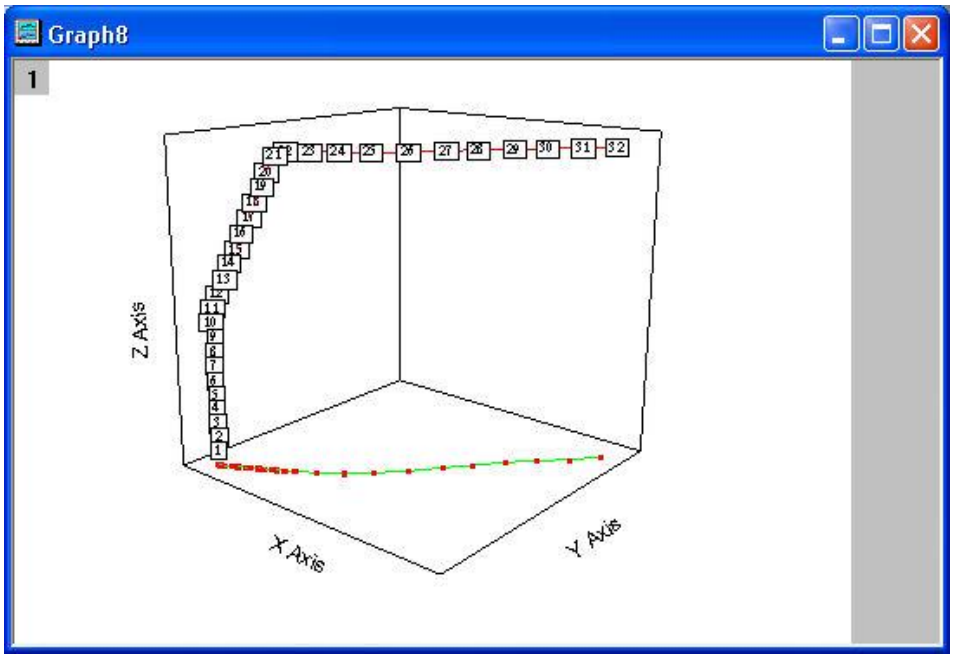


Figure 13. A formatted 3D plot

The 3D Rotation toolbar (see Figure 39) has several buttons that can be used to rotate and change the perspective of the 3D graph. The six buttons on the left rotate and tilt the 3D plot by the specified rotation angle, in this case 10°. The next two increase and decrease the perspective angle by 3°. The last two fit the graph to the layer frame and reset the rotation angles. If the 3D Rotation toolbar is not displayed, open it by selecting **View > Toolbars** and then 3D Rotation.

Figure 14. The 3D Rotation toolbar

Task 12 Creating a surface graph

Objective To create a surface graph from 3D data stored in a matrix sheet.

Instructions You will create matrix sheet data from worksheet data and plot it as a 3D surface graph.

Surface graphs can only be plotted from matrix sheet data in matrix book windows. Matrix sheet data can be input in several ways: it can be created from a formula; copied and pasted from another application; imported; or created from an existing worksheet as in the following example.

Activity 12.1 To try this example:

- Open a new workbook and import the ASCII data file XYZ Random Gaussian.dat from Q:\origin8.v01\Samples\Matrix Conversion and Gridding (as in Activity 7.1).

The worksheet displayed should have three columns A(X), B(Y) and C(Y).

- Change the association of column C to Z (as in Activity 11.1).

Activity 12.2 To create matrix sheet data from this worksheet data:

- Highlight column C(Z) and select **Worksheet > Convert to Matrix > XYZ Gridding**.
- Select the Random (Kriging Correlation) gridding method in the XYZ Gridding dialog box which appears.

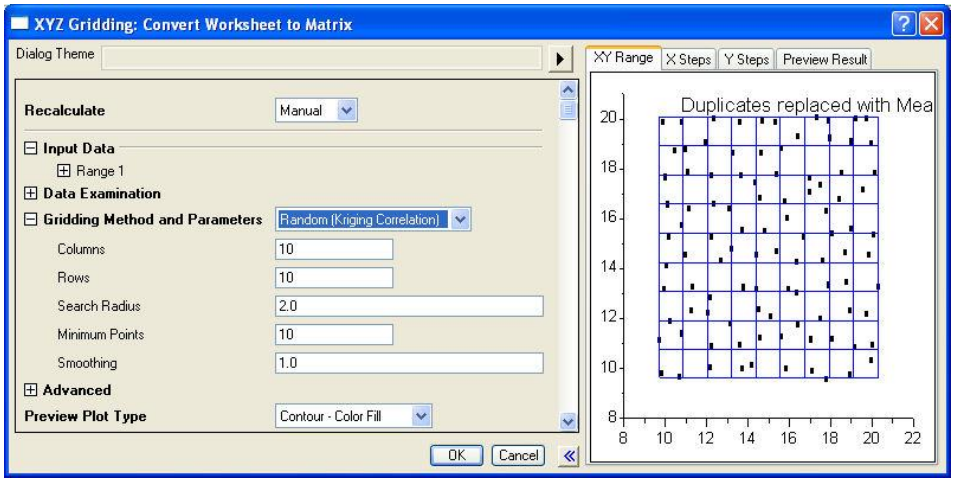


Figure 15. The XYZ Gridding dialog box

Activity 12.3 You can now select values for the following gridding parameters: number of columns and rows; search radius; minimum number of points; and amount of smoothing required for the data. The values selected will determine how fine/blocky any graph created will be. From your XYZ data, OriginPro will interpolate values for each cell in the matrix sheet - the more cells, the finer any graph created will be, but too many cells will take much longer to

calculate and could be meaningless if there is not sufficient data. The search radius value is used to determine which of your XYZ data points will be used to compute each cell value - this needs to be big enough to cover small gaps in the data but should not be so big that values at one end of the dataset have an effect at the other end.

If you are not sure about values for your dataset, try several different ones. For this example:

- Accept the default values and click on OK.

The matrix sheet data in Figure 41 is created.

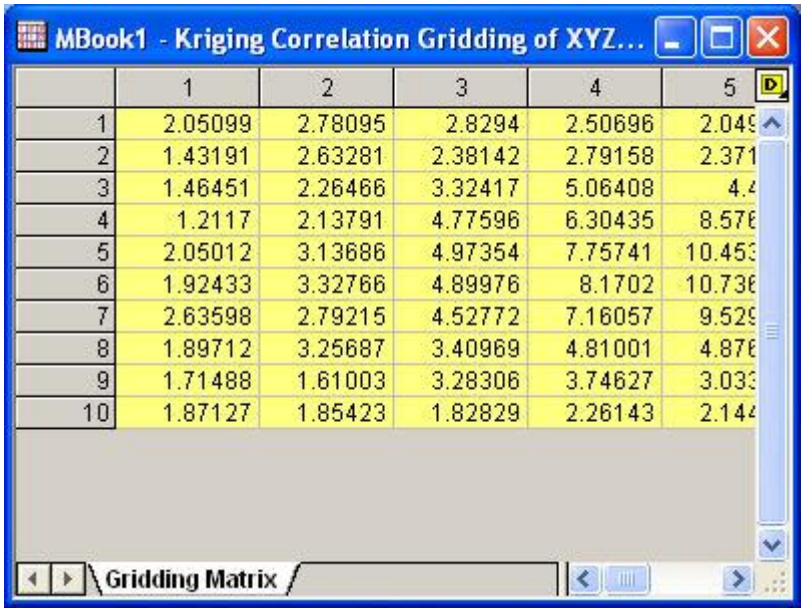


Figure 16. The matrix book window

Activity 12.4 You are now ready to plot the surface graph.

- Open the **Plot** menu and click on the **3D Surface > Color Map Surface** option.

The surface graph which is plotted is shown below.

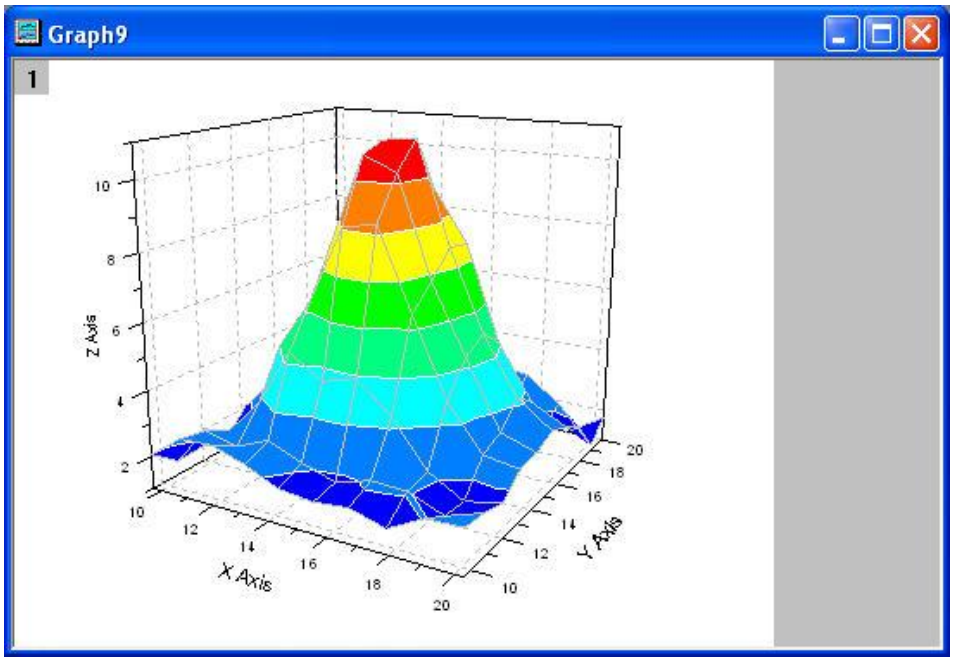


Figure 17. A colour map surface graph

- Now open the Plot Details dialog box by double-clicking on one of the grid data points.

If the matrix sheet data is not selected on the left-hand side of the Plot Details dialog box, expand Layer1 by clicking on the + symbol and then select it.

- Most of the options are self-explanatory so try and play around with them, especially experimenting with the plot type options at the bottom left of the dialog box.

Task 13 Quitting OriginPro

Objective To quit OriginPro.

Instructions You will use the **Exit** option from the **File** menu.

Activity 13.1 To quit OriginPro:

- Select the **Exit** option from the **File** menu.

Note: If you have not saved the project, you are now given the opportunity to do so before exiting.

Further information

Documentation

To find out more about OriginPro 8, the *Origin 8 User Guide* is available for reference or loan from the ISS Help Desk.

This manual can also be purchased directly from Silverdale Scientific for £25 (e-mail **sales@silverdalescientific.co.uk**) or downloaded for free as a pdf file, *Origin_8_User_Guide.pdf*, from the OriginLab website (**http://www.originlab.com/index.aspx?s=12&lm=66**), along with documentation for previous versions.

There are also the following manuals available for previous versions of the software from the ISS Help Desk:

Getting Started Manual

Microcal Origin 3D/Contour Manual

Microcal Origin LabTalk Manual

Microcal Origin User's Manual

Peak Fitting Module Manual

Programming Guide

Help

OriginPro incorporates a built-in help system which includes a search facility. You can access help by choosing one of the options from the **Help** menu.

You can also contact the ISS Help Desk if you have any questions about using OriginPro (e-mail **helpdesk@leeds.ac.uk** or phone 0113 34 33333).

Appendix 1 Types of graph available under the Plot menu

For workbook windows:

Line

Line
Horizontal Step
Vertical Step
Spline

Symbol

Scatter
Y Error
XY Error
Vertical Drop Line
Bubble
Color Mapped
Bubble + Color Mapped

Line + Symbol

Line + Symbol
Line Series
2 Point Segment
3 Point Segment

Columns/Bars

Column
Bar
Stack Column
Stack Bar
Floating Column
Floating Bar
Pie

Multi-Curve

Double-Y
Stack Lines by Y Offsets
Waterfall
Vertical 2 Panel
Horizontal 2 Panel
4 Panel
9 Panel
Stack

3D XYY

3D Waterfall
3D Walls
3D Ribbons
3D Bars

3D XYZ

3D Scatter
3D Trajectory

Statistics

Box Chart
Histogram
Histogram + Probabilities

Stacked Histograms

QC (X Bar R) Chart

Scatter Matrix

Area

Area

Fill Area

Contour

XYZ Contour

theta(X) r(Y) Z Polar Contour

r(X) theta(Y) Z Polar Contour

Specialized

Polar theta(X) r(Y)

Polar r(X) theta(Y)

Ternary

Smith Chart

High-Low-Close

Vector XYAM

Vector XYXY

Zoom

For matrix book windows:

3D Surface

Color Fill Surface

X Constant with Base

Y Constant with Base

Color Map Surface

3D Wires and Bars

Wire Frame

Wire Surface

Bars

Statistics

Histogram

Contour

Contour - B/W Lines + Labels

Gray Scale Map

Contour - Color Fill

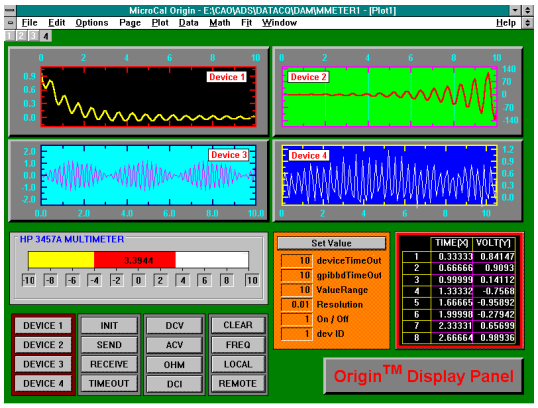
Profiles

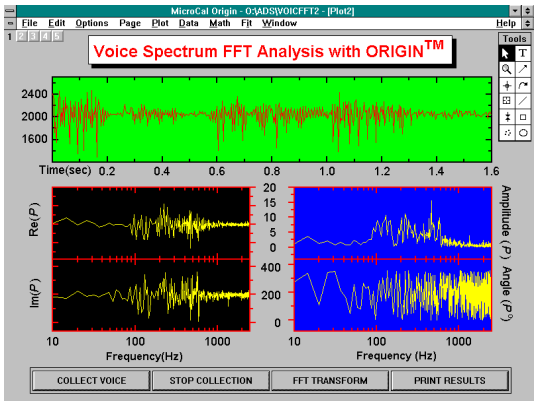
Image

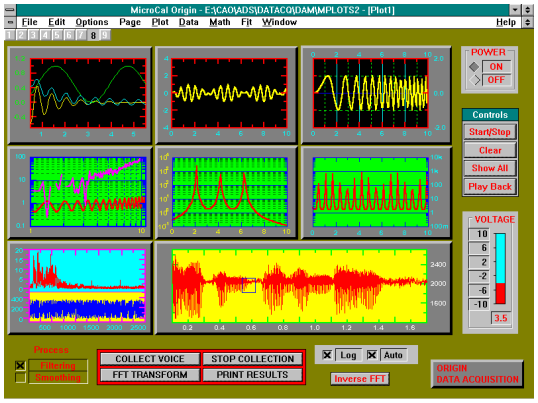
Image Plot

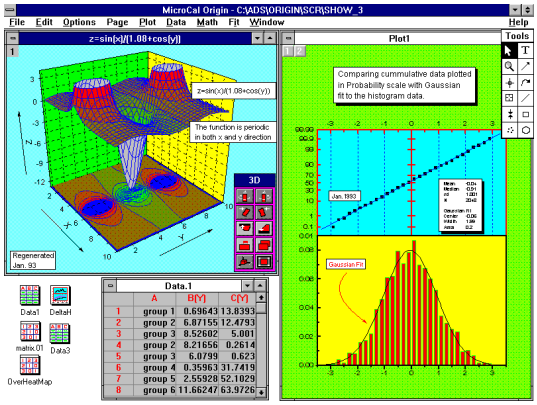
Profiles

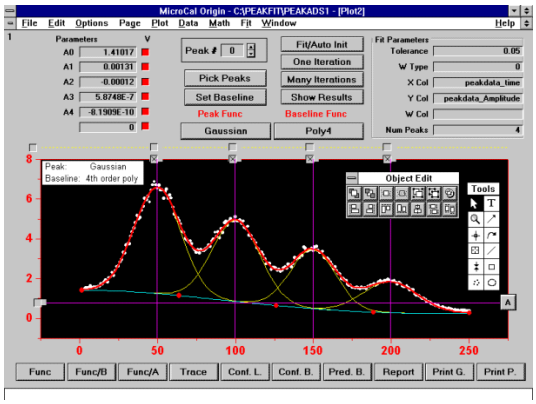
Appendix 2 OriginPro examples

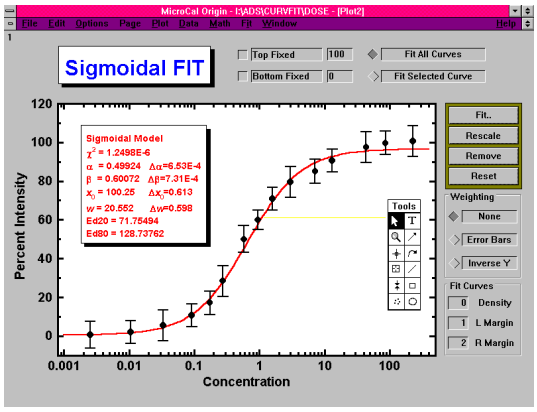


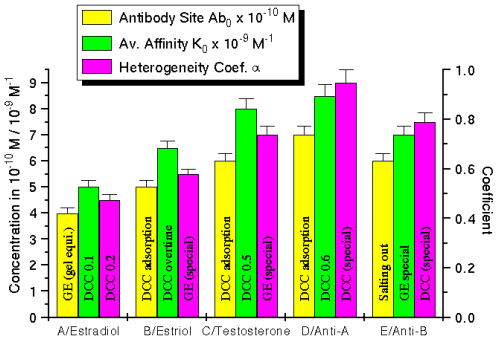


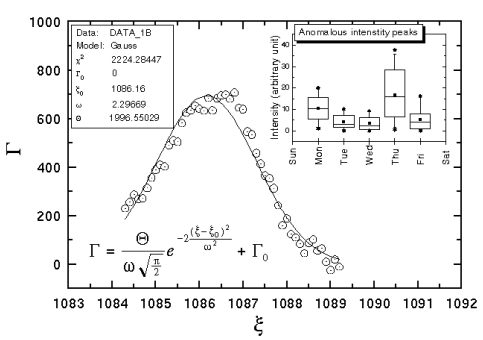












An introduction to OriginPro, a scientific charting package.